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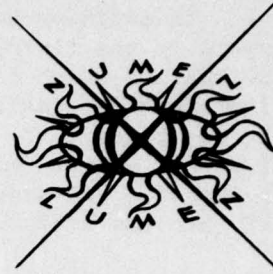YEAR 1978,

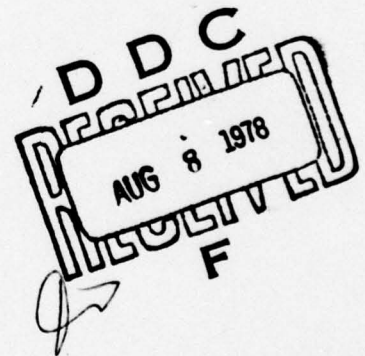April 1, 1978 through June 30, 1978.

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ANALYSIS OF EVOLUTIONARY ERROR IN FINITE
ELEMENT AND OTHER METHODS

M. J. P. Cullen[1] and K. W. Morton[2]

Technical Summary Report #1832
February 1978

ABSTRACT

Restriction and prolongation operators are used to provide a unified frame-work for the discussion of errors in approximating evolutionary equations. A generalized truncation error enables the spline-Galerkin method to be studied in detail and the accuracy of various treatments of non-linear terms (such as the advection operator $\underline{v} \cdot \underline{\nabla} v$) compared: it is shown how a multi-stage Galerkin pro-cess can give errors which are $O(h^{2l})$ for splines of order ν and quite general differential operators. A Petrov-Galerkin method is derived for $\lambda_t = a^2 u_x$ which is accurate and stable.

SIGNIFICANCE AND EXPANATION

Most problems in continuum mechanics (fluid flow, combustion, elasticity) involve partial differential equations that can be solved only numerically by computer. Originally most numerical methods for this class of problem used finite differences, which involve direct replacement of derivatives by difference formulae. In the last ten or fifteen years, finite element methods have become increasingly popular. These involve starting from an assumed functional form for the unknowns (e.g. piecewise polynomial), then determining parameters in the func-tional representation via satisfying the partial differential equation in some approximate sense.

As finite element methods become increasingly used for non-steady problems, it becomes important that their performance can be compared in detail with that of the longer established finite difference methods. This paper sets up a frame-work in which this can be done. Analysis of the spline-Galerkin methods is carried out and highly accurate schemes put forward for the advection operator $\underline{v} \cdot \underline{\nabla} v$, which occurs in the equations for practical problems in which motion of fluid and material particles are involved.

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A SET OF ORTHOGONAL POLYNOMIALS THAT GENERALIZE

THE RACAH COEFFICIENTS OR 6 - j SYMBOLS

Richard Askey[1] and James Wilson

ABSTRACT

A very general set of orthogonal polynomials with five free
parameters is given explicitly, the orthogonality relation is
proved and the three term recurrence relation is found.

SIGNIFICANCE AND EXPLANATION

Orthogonal polynomials are used in numerical analysis for interpolation

and quadrature, in the quantum mechanical theory of angular momentum, in

statistics and many other areas. The polynomials introduced in this paper

contain all the classical orthogonal polynomials as limits, and so provide

a unified way of deriving some of the properties of the classical polyno-

mials, as well as giving us a more general set of polynomials to use for

applications.

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THE USE OF STOCHASTIC PROGRAMMING FOR THE SOLUTION

OF SOME PROBLEMS IN STATISTICS AND PROBABILITY

András Prékopa

Technical Summary Report #1834
March 1978

ABSTRACT

The applicability of known stochastic programming models and

methods for the solution of problems in classical statistics and

probability is shown by a number of examples. These concern testing

of hypotheses, constructing of tolerance regions, planning of optimal

sampling and the Moran model for the dam.

SIGNIFICANCE AND EXPLANATION

Mathematical programming deals with optimization under constraints, e.g.

minimization of costs in manufacturing operations when sources of supply,

machines and manpower are limited. Stochastic programming deals with

mathematical programming problems in which there is uncertainty associated

with the variables and with the constraints in the optimization problem. Thus

stochastic programming lies on the borderline between mathematical programming

and statistics. However, the connection between the development of these two

sciences is not strong enough.

The purpose of this paper is to show how some stochastic programming

methods (developed by the author) can be applied in classical problems of

statistics. Models are formulated for a) construction of statistical

tests, b) construction of tolerance regions, c) optimum allocation in

surveys, d) the dam problem of MORAN. The solution of the above problems

uses nonlinear programming combined with simulation. Evidence concerning

effective solvability of such problems is given in other referenced papers.

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PLANNING IN INTERCONNECTED POWER SYSTEMS:
AN EXAMPLE OF TWO-STAGE PROGRAMMING UNDER UNCERTAINTY

András Prékopa

Technical Summary Report #1835

March 1978

ABSTRACT

The problem of planning in interconnected power systems is formulated as a stochastic programming model, a variant of the model: two stage programming under uncertainty. In our case the solvability of the "second stage problem" is required only for a probability near unity.

SIGNIFICANCE AND EXPLANATION

Mathematical optimization techniques are now widely used in business, government service, and the armed forces. A typical problem involves finding the cheapest method of providing certain services, using various available sources of supply, under given constraints, e.g. on the level of production of individual sources. Problems where we know exactly the sources of supply and their limitations, are called deterministic. Such problems have led to intensive development of mathematical optimization techniques such as linear and nonlinear programming.

In most situations there is some uncertainty as regards the sources of supply and their limitations. Such problems are called stochastic. They have received much less attention than deterministic problems, partly because they are much more difficult.

The type of problem considered in this paper will be described in terms of electrical power systems; it should be clear that the model covers very many other situations. Suppose that the power systems are interconnected so as to form a network. If a system cannot serve the demand of its own area because of (random) excess demand and/or (random) deficiency in the electricity generation, then the other systems help to meet the total demand. How can we design the cheapest possible system so as to reach a prescribed (high) reliability level?

The problems considered in this paper are based on the following underlying deterministic model:

$$\text{Minimize } (c'u + d'v)$$

$$\text{subject to } Au \geq b,\ Tu + Mv \geq \xi\ .$$

When the ξ is assumed to be random, the model is formulated as a two-stage problem in which we first decide on u, then choose the random variable ξ, then find v. The variable u represents supply, ξ represents random demand plus deficiency in various areas, and v represents dispatch power.

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SOME OPTIMAL PROPERTIES AND INTERPRETATIONS OF PRINCIPAL COMPONENTS

Raul Hudlet and Richard A. Johnson

ABSTRACT

Optimal properties are derived and some new geometrical interpretations given for principal components. Typically, our main results concern the simultaneous minimization of eigenvalues of certain covariance matrices which measure the goodness of an approximation. Many popular criteria like total variance and generalized variance, which are increasing functions of the eigenvalues, are then minimized by the best approximator.

In other situations, the criterion may not be a monotone function of the eigenvalues. In Theorem 3.2, we derive a general optimal class based on the non-negative definite ordering of covariance matrices.

Theorem 4.1 gives a result for the sequential selection of principal components. In the final section, we give a new geometrical interpretation of the sample principal components.

SIGNIFICANCE AND EXPLANATION

When a large number of characteristics are measured on a large number of population units, the sheer volume of data can cause problems. It is natural, in such cases, to look for ways to reduce that data to a more manageable form.

One way of doing this is the Principal Component Method, wherein the original problem is replaced by an approximation of far lower dimension. The variables in the approximate problem are certain linear combinations, or principal components, of the variables in the original problem.

Of course, some choices of the exact linear combinations to be used (approximators) will yield more meaningful results than others. Ideally, we would like to retain as much information as possible, and we seek a set of principal components which is optimal from this point of view.

In this paper, we derive some new properties of optimal principal component approximators and obtain some further geometrical insights concerning this method. We also help clarify a potential weakness in this method by determining an even more general class of approximators, that contains those selected by the principal component, and exhibiting a situation where the approximator that would be selected by that method is not optimal.

ABSTRACT

The analysis of linear models with independent homoscedastic, normal noise (white noise) occupies a prominent position in applied statistics. This report is concerned with the linear model analysis of data which cannot be assumed statistically independent because the data have been collected sequentially in time or space.

Assuming that the noise in a linear model (with p-dimensional parameter vector β) follows a first order autoregressive scheme (with parameter ϕ), it is shown in Chapter 2 how in the Bayesian framework inferences can be drawn about β and ϕ jointly, conditionally and marginally. Two AR-1 schemes are considered, one covering explosive as well as stationary situations, the other assumes stationarity and reversibility a priori. The important task of choosing an appropriate joint prior distribution for the parameters is given special attention.

Recognizing that the assumption of independence can be a crucial one, it has become a widespread practice in such regression work, where observations are made in time order, to test for serial correlation using the well known Durbin-Watson test. This test corresponds to determining whether a certain estimate $\hat{\phi}$ of ϕ is significantly different from zero. It is shown in Chapter 3 that only in relation to a model lacking a mean do suggested alternative testing procedures show decisively greater empirical power than the DW-test. However it is argued that tests of a null hypothesis of independence should really not be carried out when serial correlation is to be expected. It is demonstrated that inferences about β may be quite misleading if made conditionally on $\phi = 0$ (when that hypothesis is "accepted") or conditionally on $\hat{\phi}$ (when it is "rejected"). The Bayesian analysis does not suffer from these handicaps. The Bayesian inference about β may be approximated by a conditional inference using the maximum likelihood estimate $\hat{\phi}$ of ϕ ($\hat{\phi}$ is found by estimating ϕ and β simultaneously by least squares), and this conditional analysis is paralleled in sampling theory framework when inferences about β are drawn as if $\phi = \hat{\phi}$.

One way in which data analysts have sometimes tried to get around the problem of dependence, is by differencing and then assuming that the errors of the differences are independent. This is equivalent to assuming that $\phi = 1$ in the AR-1 noise model, and the plausibility of this particular value for ϕ may be assessed by studying the marginal posterior distribution of ϕ. For models involving a mean this parameter vanishes for $\phi = 1$. This creates a singularity, and it is shown in Chapter 4, how the density may be found at such (distinct) points. It is also developed in the Bayesian framework, how the appropriateness of differencing may be assessed using posterior model probabilities for two alternative noise models, one assuming the original observations to have AR-1-noise, the other that the differences have AR-1 noise.

SIGNIFICANCE AND EXPLANATION

One of the most widely used statistical techniques in applied fields like

engineering, business, economics, sociology etc. is linear model analysis

(analysis of variance, regression analysis, etc.). When the data to be analyzed

are collected sequentially in time or space, it turns out, more often than not,

that the data at any given point in space or time depend to some extent on the

data at neighboring points in space or in instants of time. The data are then

said to be serially correlated (autocorrelated). However "standard" methods of

analysis usually assume the observations to be statistically independent; if the

assumption of independence is incorrect, this will invalidate the analysis and

may cause very misleading conclusions.

This report is devoted to studying how serially dependent data may be

analyzed, when one extra parameter is incorporated to allow for serial correla-

tion. Specifically it is developed in the Bayesian framework how general linear

models may be analyzed when the noise follows a first order autoregressive process

(a Markov process). We argue against following the popular practice of checking

independence with a Durbin-Watson test whenever serial correlation is feared.

One way to get around the problems of serial correlation which has some-

times appeared helpful is to difference the series, i.e. analyze the increments

rather than the original data. The question of whether to difference or not to

difference is looked into in a quantitative way.

STUDIES I: THE ANALYSIS OF SERIALLY DEPENDENT DATA

Lars Chr. Pallesen

#1837

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UNIQUENESS OF SOLUTIONS TO HYPERBOLIC CONSERVATION LAWS

Ronald J. DiPerna

Technical Summary Report #1838
March 1978

ABSTRACT

We study strictly hyperbolic systems of conservation laws.
We consider the class K of solutions which lie in $L^\infty \cap BV$
and satisfy the entropy admissibility criterion. We show under
certain hypotheses that admissible piecewise Lipschitz solutions
are unique within K. We establish the L^2-stability of classical
solutions relative to perturbations in K and we show that admissible piecewise Lipschitz solutions to the quasilinear wave equation satisfy the entropy rate criterion relative to a broad subclass of solutions in K.

Subject Matter Classification: 35L60, 35L65

Key Words: Hyperbolic conservation laws,
initial value problem,
entropy inequality

Work Unit Number 1 - Applied Analysis

SIGNIFICANCE AND EXPLANATION

It is known that conservative systems of differential equations which
result from continuum mechanics (e.g. the equations of shallow water waves,
fluid dynamics, magneto-fluid dynamics and certain elasticity problems) do
not have unique solutions. Thus the problem arises of proving that systems
of this type have only one physically meaningful solution. In this report
we show that there exists at most one solution satisfying an entropy condition which generalizes the second law of thermodynamics.

The responsibility for the wording and views expressed in this descriptive
summary lies with MRC, and not with the author of this report.

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QUADRATIC INTERPOLATION IS RISKY

Stephen M. Robinson

Technical Summary Report #1839

March 1978

ABSTRACT

This brief note points out that the method of quadratic interpolation,
which has been recommended in the literature for minimizing a function of one
variable, can be very undependable. In particular, unless the function being
minimized is itself quadratic, the method may break down no matter how close
to the minimizer one starts.

SIGNIFICANCE AND EXPLANATION

In many practical applications we have to find numerically the minimum
or maximum value of a function of one variable: an example might be a
statistical estimation problem in which we try to find the value of a parameter
which maximizes the likelihood function.

A simple method which has been recommended in the literature is to find
the function values at three distinct points, then fit a quadratic function
(a parabola) to these. The maximum or minimum value of this quadratic function
is then found, together with the point at which it is attained, and this point
is used together with two of the original three points to repeat the process.

This note points out that unless the function being minimized is itself
quadratic, the above algorithm may break down (the new point may be one of the
original three even though none of these minimizes the function). Even if the
method does not break down, it may provide inaccurate answers because of the
effects of roundoff error. Thus, it could be unwise to use this method.

The responsibility for the wording and views expressed in this descriptive
summary lies with MRC, and not with the author of this report.

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BAYESIAN INFERENCE ON PARAMETERS ASSOCIATED WITH FAMILIES CLOSED UNDER RECIPROCATION*

Norman R. Draper and Irwin Guttman**

ABSTRACT

Recently, Saunders 1974 has generalized the so-called reciprocal property for normality. Distributions having this property are called ξ-normal, and it is of interest to make statistical inferences about the relevant parameters when sampling from such a distribution. Previous work on such problems has been from the sampling viewpoint.

In this paper, we approach the inference problem from the Bayesian point of view and investigate the posterior of the parameters involved when sampling is from the ξ-normal with parameters α and β. Two special cases are examined, $\xi(v) = \log_e v$, which gives rise to the lognormal distribution, and $\xi(v) = v^{1/2} - v^{-1/2}$, a case that arises in certain fatigue problems (Saunders and Birnbaum 1969).

AMS (MOS) Subject Classification: 62F15

Key Words: ξ-normal distribution; characteristic life; posterior distributions; posterior intervals; estimation

Work Unit Number 4 (Probability, Statistics, and Combinatorics)

SIGNIFICANCE AND EXPLANATION

Statistical problems involving "time to failure", "strength of material", and "fatigue" are often characterized by a statistical distribution known as the lognormal distribution; the length of life of a system subjected to fluctuating stresses by a periodic loading can sometimes be predicted through the use of the Birnbaum-Saunders life length distribution.

These distributions are special cases of a more general class of distributions based on certain functions $\xi(t)$, that map $0 \le t \le \infty$ into $-\infty \le \xi(t) \le \infty$ and have the property that $\xi(t) = -\xi(1/t)$. In the above cases, we have $\xi(t) = \ell n\, t$ and $\xi(t) = t^{1/2} - t^{-1/2}$, respectively.

A random variable T is said to be ξ-normally distributed if $\xi(T/\beta)/\alpha = Z$, where Z is distributed normally with zero mean and unit standard deviation; α and β are the parameters of the ξ-normal distribution. Given a set of data values $t_1, t_2, \ldots, t_n$, we would like to be able to make inferences about the values of the parameters α and β. In this paper, we approach this problem via Bayesian methods.

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ON THE RELATIONSHIP OF SOME RESULTS OF GELFAND-DIKII
AND P. MOERBEKE, AND A NATURAL TRACE FUNCTIONAL
FOR FORMAL ASYMPTOTIC PSEUDO-DIFFERENTIAL OPERATORS

M. Adler

Technical Summary Report #1841
April 1978

ABSTRACT

This paper developed out of an attempt to understand results of Gelfand-Dikii [1] and P. Moerbeke (unpublished version of [2]) in a unified way. We provide a natural abstract setting for understanding the symplectic structure involved in both results. The setting is an orbit in the dual algebra of a group. We also discuss a natural trace functional for formal asymptotic pseudo-differential operators. In addition we discuss so-called Lenard recursion relations inherent in these structures.

SIGNIFICANCE AND EXPLANATION

It is one thing to write down the equations governing the behavior of a physical system in time; it is quite another thing to solve them. Historically, an important step forward in explaining the behavior of mechanical systems was made when it was realized that, for some systems, certain quantities like energy and angular momentum were independent of time, i.e. invariant. This is a tremendous help in solving the equations both analytically and numerically, since the invariants are equivalent to first integrals of the equations of motion, and constrain the class of functions within which we need look for solutions.

It turns out that in many problem of physical interest involving partial as well as ordinary differential equations, it is possible to find a denumerable number of quantities that are invariant as time evolves. This paper gives a unified method for finding invariants for a class of equations that includes crystal lattices (the Toda equations), stochastic processes (Kac-Moerbeke), and water waves (Boussinesq and Korteweg-deVries). In addition, the mechanical structure of these systems, as discovered by respectively Gelfand-Dikii, and P. Moerbeke are given geometrical significance.

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ON THE DEVELOPMENT OF OPTIMIZATION THEORY

András Prékopa

Technical Summary Report #1842
April 1978

ABSTRACT

The method of Lagrange for finding extrema of functions subject to equality
constraints was published in 1788 in the famous book Mécanique Analytique. The
works of Karush, John, Kuhn and Tucker concerning optimization subject to inequality
constraints appeared more than 150 years after that. The purpose of this paper is
to call attention to important papers, published as contributions to mechanics, con-
taining fundamental ideas concerning optimization theory. The most important works
in this respect were done primarily by Fourier, Cournot, Farkas and further by Gauss,
Ostrogradsky and Hamel.

SIGNIFICANCE AND EXPLANATION

This is a historical paper. It concerns the necessary conditions of
optimality for nonlinear optimization.

The solution of nonlinear programming problems is based on the neces-
sary conditions formulated for the case of equality constraints by Lagrange
in 1788 and for the case of inequality constraints by several authors
between 1939 and 1950 (Karush, John, Kuhn, Tucker). This paper tries to
complete the general historical picture by showing that, in the form of
contributions to mechanics, the basic ideas were already discovered jointly
by Fourier, Cournot and Farkas, among others.

Many referenced papers are thoroughly analyzed.

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TESTING FOR PERIODICITY IN A
TIME SERIES[+]

Andrew F. Siegel

Technical Summary Report #1843
April 1978

ABSTRACT

In 1929, Sir R. A. Fisher proposed a test for periodicity in a time series
based on the maximum spectrogram ordinate. In this paper I propose a one-
parameter family of tests that contains Fisher's test as a special case. It is
shown how to select from this family a test that will have substantially larger
power than Fisher's test against many alternatives, yet will lose only negligible
power against alternatives for which Fisher's test is known to be optimal. Criti-
cal values are calculated and tabled using a duality with the problem of covering
a circle with random arcs. The power is studied using Monte Carlo techniques.
The method is applied to the study of the magnitude of a variable star, showing
that these power gains can be realized in practice.

SIGNIFICANCE AND EXPLANATION

An important problem in the analysis and prediction of physical systems
is answering the question "is there periodicity?" when the measurements of its
evolution through time contain a random element. Periodicity refers to the
regular repetition of a pattern as, for example, with the eleven year cycle
of the sun. Problems of this type have often arisen in meteorology, astronomy,
and other sciences, and in 1929, Sir R. A. Fisher proposed a statistical test
designed for this situation.

In this paper, new statistical procedures are proposed for this problem
that represent a generalization of and an improvement upon Fisher's test.
The improvement is in the power of these tests: they are more sensitive to
the detection of certain types of periodicity without sacrificing overall
sensitivity. The procedure is readily applied to data. Instructions and tables
as well as theory and examples are included in the report.

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A THEORY FOR IMPERFECT BIFURCATION
VIA SINGULARITY THEORY

M. Golubitsky* and D. Schaeffer**†

Technical Summary Report #1844
April 1978

ABSTRACT

In this paper we apply the theory of singularities of differentiable mappings - specifically the unfolding theorem - to study the effect of imperfections in a system subject to bifurcation. In a number of special cases we have classified (up to a suitable equivalence) all the possible perturbations of the bifurcation equations by a finite number of imperfection parameters. These cases include both bifurcation from a double eigenvalue and from a simple eigenvalue degenerate in the sense of Crandall-Rabinowitz.

AMS(MOS) Subject Classifications: 58F99, 35B30.

Key Words: Bifurcation theory, Imperfections, Singularity theory.

Work Unit Number 1 - Applied Analysis

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SIGNIFICANCE AND EXPLANATION

Bifurcation theory is concerned with the appearance of multiple solutions to the equations governing the equilibria of a physical system as a parameter is varied. The most familiar example of this theory concerns the buckling of a beam as the compressive load is increased (so-called Euler buckling) - for small loads the undeflected state is the only solution of the governing equations; for larger loads solutions with deflection also exist, and are in fact preferred by physical systems, from considerations of stability.

It is widely recognized that small imperfections in a system may have a profound influence on its bifurcations. For instance, in the idealized treatment of the beam problem above, the theory predicts that upwards and downwards deflections are equally probable, but in experiments specimens will buckle repeatedly in the same direction because of small imperfections in the experiment which destroy the symmetry between up and down. Also the experimentally measured buckling loads for beams are dramatically less than predicted by the idealized theory. Although many attempts have been made to explain its phenomenon, no universally accepted explanation has so far been produced.

It is well known that sensitivity to imperfections is greatly increased when a system loses stability in situations where there are two buckling modes present simultaneously - i.e. bifurcation from a double eigenvalue.

In this paper we use the theory of singularities of differentiable mappings to study bifurcation in the presence of imperfections. In a number of important special cases, including some bifurcations from a double eigenvalue and some bifurcations from a simple eigenvalue degenerate in the sense of Crandall-Rabinowitz, we have classified all the possible perturbations of the given problem. The classification depends on a (small) finite number of imperfection parameters.

The most promising applications of the theory concern bifurcation from a double eigenvalue. We have already analyzed bifurcations near a double eigenvalue of the equations governing certain model chemical reactions with these techniques, and we anticipate other applications, specifically to mode jumping in buckled plates and to the selection of the number of cells in the Taylor fluid instability problem in a cylinder of finite length.

SIGNIFICANCE AND EXPLANATION

In the analysis of such nonlinear problems as the melting (Stefan) problem and the filtration of water through a porous dam, it is important to know whether small changes in the physics of the system produce large changes in the physical end-results. When the system is modelled mathematically this means that we have to study the behavior of some associated nonlinear operator.

This is done by establishing a measure of the effect of small changes in the parameters in the problem (a topology). It turns out that in the two physical problems mentioned above, the nonlinear operators involved are monotone.

Roughly speaking "$F(x)$ monotone increasing" means that an increase in x produces an increase in $F(x)$. In many situations, monotonicity of the operators involved guarantees that the corresponding physical problems are well-behaved, and guarantees convergence of numerical methods for solving these problems. Another important class of well-behaved operators are those arising from so-called affine mappings, i.e. linear operators plus a displacement.

The question naturally arises as to whether there are any other well-behaved classes of operators. In this paper the question is answered in the negative: if a given operator is well-behaved (e.g. in the sense that it has certain convergence properties) then it must be either monotone or affine.

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MONOTONICITY IS NECESSARY AND SUFFICIENT
FOR COMPENSATED COMPACTNESS

Robert Jensen

Technical Summary Report #1845
April 1978

ABSTRACT

Let $F : R^n \to R^n$ be a continuous map and set
$$G_F \equiv \{v \in W^{1,\infty}(R^n) \mid \text{div}(F(\nabla v)) = 0\}.$$ The function F gives rise to a map
$$T_F : G_F \to (L^\infty(R^n))^n \text{ via } T_F : v \to F(\nabla v).$$
We show that if T_F is continuous (for the w^* topologies on G_F and $(L^\infty(R^n))^n$) then F is either affine or monotone.

AMS (MOS) Subject Classification: 47H05

Key Words: Monotonicity, w^* topology, Affine map, Affine subspace

Work Unit Number 1 (Applied Analysis)

INVERSE BOUNDARY VALUE PROBLEMS
AND A THEOREM OF GEL'FAND AND LEVITAN

W. Symes

ABSTRACT

This report concerns two so-called inverse problems of mathematical physics. These are: (i) the problem of determining a second-order differential operator (in a normal form) on the half-axis from its spectral function; and, (ii) the problem f determining a hyperbolic boundary value problem of a special form in a (non-characteristic) half-plane from its response on the boundary to a unit impulse at some reference time $t = 0$ (boundary value of the Riemann function).

We solve problem (ii) by a natural approach, and then indicate how the solution of problem (i) follows from the solution of problem (ii). Our solution of problem (ii) is constructive, and we obtain stability of the solution under perturbation of the data, in a well-defined sense.

For problem (i), we obtain the well-known result of Gel'fand and Levitan, in the sharp formulation given by Levitan and Gasymov ([6]).

AMS(MOS) Subject Classification - 35R30

Key words: Inverse problem
Hyperbolic boundary value problem
Nonlinear Volterra equation
Gel'fand-Levitan theorem

Work Unit No. 1 - Applied Analysis

Significance and Explanation

This report concerns an inverse problem of wave propagation. In general, inverse problems for dynamical systems require that the dynamical laws of a system be recovered from information about the behaviour of the system, such as its response to a specific stimulus, or its long-time asymptotic behaviour. Direct problems of dynamical systems, which require that the behaviour of a system be calculated from the dynamical laws, assumed known, have a long history, and comprise the bulk of classical mathematical physics. Of course our understanding of physical systems proceeds by the solution of inverse problems; we observe the behaviour of a system, and try to infer its dynamics. Nevertheless, such inverse problems are usually approached by a sequence of guesses about the dynamical laws perhaps with some free parameters followed by solutions of the corresponding direct problem, and attempts to adjust the free parameters so that the predicted behaviour of the system matches its observed behaviour. Frontal attacks on specific inverse problems, on the other hand, have been relatively rare.

In this report, we consider a very simple model inverse problem of wave propagation in a one-dimensional inhomogeneous medium. Examples of physical problems to which our methods apply are: (i) the description of the (inhomogeneous) density distribution of a vibrating string from observation of the motion of one point along its length; (ii) synthesis of a cable of a restricted type, having prescribed transmission characteristics for signals of various frequencies.

In actual applications, stability is an important attribute of any computation scheme. One wants to ensure that small errors in the input data do not result in huge, uncontrollable errors in the solution; otherwise, the scheme is generally useless. We show that our reconstruction of the dynamical law of our simple model system is stable, in a precise sense, against small perturbations of the "observed" data; in fact, we give an approximation scheme with explicit error bounds.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the author of this report.

ABSTRACT

A Poisson structure (antisymmetric bilinear local operator on functionals, obeying the Jacobi identity) is established on certain function spaces (spaces of symbols of pseudodifferential operators on R^n. The spaces of functionals thus become (infinite-dimensional) Lie Algebras. This type of Lie algebra structure has been established previously for functionals of a single variable (n = 1) only. For n = 1, the theorem of Gardner, as generalized by Gel'fand, Dikii, and others, is proved: that is, the residues of the zeta-function of the elliptic symbol

$$\xi^{m+2} + \sum_{j=0}^{m} g_j(x)\xi^j$$

are in involution with respect to the appropriate Poisson bracket. In contrast, it is shown by explicit example that the residues of the zeta functions of higher-dimensional elliptic symbols are generally not in involution.

SIGNIFICANCE AND EXPLANATION

In recent years several nonlinear partial differential equations of applied mathematics have been discovered to have the extraordinary property known as complete integrability: that is, roughly speaking, they possess the maximum number of constants of motion possible for the type of system considered. These equations arise in the study of shallow water waves, accoustic waves in plasmas (Korteweg-deVries equation) nonlinear optics, Josephson junction theory, (sine-Gordon equation), other plasma phenomena (nonlinear Schrödinger equation), and other areas. The complete integrability property - again, roughly speaking - allows unusually explicit solution of these equations.

This report is concerned with two other noteworthy properties of these equations. First, all of the above-mentioned partial differential equations involve only two independent variables, hence model systems whose spatial variation is essentially restricted to a single linear dimension: one independent variable thus represents space (location), and the other variable represents time, in applications. Second, each of the above-mentioned examples is, in some sense, a Hamiltonian system. Hamiltonian systems commonly occur in mechanics (both classical and quantum), and are characterized by the existence of special coordinates, called canonical coordinates, in the state space of the system, in which the equations of motion take a particularly simple form, called Hamilton's Equation. The examples of the first paragraph belong to continuum mechanics, hence manifest infinitely many degrees of freedom. Nonetheless, a set of canonical coordinates (infinitely many, of course) may be chosen for each of those examples, so that each partial differential equation, expressed in terms of these special coordinates, becomes a Hamilton's equation. It should be remarked that Hamiltonian systems are very special dynamical systems.

An obvious question is, whether the phenomenon represented by the examples of the first paragraph is somehow restricted to partial differential equations in two independent variables - or, in terms of applications, to systems with (essentially) one linear dimension. In approaching this question, one may choose to emphasize some aspects of the phenomenon over others. In this report, we concentrate on the Hamiltonian structure suggested by our examples, especially the Korteweg-deVries equation. We show that the Hamiltonian structure is independent of the number of spatial dimensions: that is, we give canonical coordinates on spaces of functions of arbitrarily many (space) variables, so that the Hamiltonian way of writing the Korteweg-deVries equation appears as a special case.

Thus Hamiltonian systems of a type represented by the examples of the first paragraph, are present in any number of (space) dimensions. In contrast, the complete integrability property (which should be considered more special than the Hamiltonian property) seems to fail in dimension greater than one. Precisely, we give an example in which the rather obvious generalizations of the constants of motion for the Korteweg-deVries equation (dim. 1) fail to be constant in dimension greater than one. This is certainly not to say that there are no partial differential equations in many independent variables which represent completely integrable Hamiltonian systems, or even that the Hamiltonian systems constructed in this paper do not have other, more cleverly chosen, constants of motion - only that the obvious choices fail to work. The significance of this apparent counterexample, and, more generally, the importance of Hamiltonian systems of Korteweg-deVries type in modeling phenomena with several independent spatial dimensions, is unclear, and suggests the need for further stud

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SOLVING DIFFERENTIAL EQUATIONS
ON A HAND HELD PROGRAMMABLE CALCULATOR

J. Barkley Rosser

Technical Summary Report #1848
April 1978

ABSTRACT

Most scientists who occasionally have to solve numerically a differential equation now own a hand held programmable calculator which will very often be adequate. Since hand held calculators are slow, there is particular need to keep the number of function evaluations to a minimum. At first thought, this would seem to rule out use of Runge-Kutta methods, but recent developments, such as those by Fehlberg (mostly unknown except to specialists), may make them competitive after all. In the area of predictor-corrector methods, some variations make excessive use of memory locations for a hand held calculator. An analysis of such matters is made in order to advise as to good procedures to follow, including alerting the solver to methods that are seldom taught in numerical analysis courses (where the emphasis is on the use of large fast computers).

AMS(MOS) Subject Classification: 34-02, 34A50, 65L05

Key Words: Runge-Kutta
predictor-corrector
numerical stability

Work Unit No. 7 - Numerical Analysis

Significance and Explanation

Until about 1950, when a scientist had to solve a differential equation numerically he had to do it by laborious use of a desk calculator. Since that time large scale computers have revolutionized the situation because they can be programmed to perform fast repetitive calculations very efficiently. In recent years hand-held calculators have come on the scene. They are adequate for many calculations, in particular for solving some kinds of differential equations. However the factors that are important for hand calculators are different from those for large scale computers. Hand calculators have only a limited number of memory locations and are comparatively slow.

When solving differential equations on a hand held calculator, there is particular need to keep the number of calculations of the function appearing in the differential equation to a minimum, else the calculation will take too long. At first thought, this would seem to rule out use of what are called Runge-Kutta methods, but some recent developments may make them competitive after all for certain types of problems. These types are identified, and a discussion, with numerical examples, is given how best to use the Runge-Kutta methods.

Some other methods which call for much fewer calculations of the function require more memory locations than are available on many hand held calculators. There still remain some methods which are modest both in the number of calculations and in memory requirements. How best to use these on a hand held calculator is explained, with numerical examples.

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ON SOLUTIONS OF NON-COOPERATIVE GAMES: AN AXIOMATIC APPROACH

Prakash P. Shenoy

Technical Summary Report #1849
May 1978

ABSTRACT

In this paper we study solutions of strict non-cooperative games that are played just once. The players are not allowed to communicate with each other. The main ingredient of our theory is the concept of rationalizing a set of strategies for each player of a game. We state an axiom based on this concept that every solution of a non-cooperative game is required to satisfy. Strong Nash solvability is shown to be a sufficient condition for the rationalizing set to exist, but it is not necessary. Also, Nash solvability is neither necessary nor sufficient for the existence of the rationalizing set of a game. For a game with no solution (in our sense), a player is assumed to recourse to a "standard of behavior". Some standards of behavior are examined and discussed.

AMS(MOS) Subject Classification: 90D10

Key Words: Non-cooperative
            Rationalizable set
            Equilibrium points

Work Unit Number 5 - Mathematical Programming and
                     Operations Research

Significance and Explanation

In this paper, we study solutions of non-cooperative games that are played just once.

A non-cooperative game consists of a set of n players, each with an associated finite set of strategies; also, corresponding to each player i there is a payoff function u_i which maps the set of all n-tuples of pure strategies into real numbers. The non-cooperative aspect of the game is that the players are not allowed to communicate with each other. This rules out collaboration or the formation of coalitions. Non-cooperative games have been used to model various situations that arise in military, political and economic contexts.

The main ingredient of our theory is the concept of rationalizing a set of strategies for every player of a game. We state an axiom based on this concept that every non-cooperative game is required to satisfy. We compare our solution with that proposed by John Nash in terms of "equilibrium points".

Not all games have solutions (in our sense). In such cases, players are assumed to have recourse to a "standard of behavior". Some standards of behavior are examined and discussed.

A COMBINATORIAL PROBLEM ARISING IN THE STUDY OF
REACTION-DIFFUSION EQUATIONS

J. Greenberg, C. Greene, and S. Hastings

ABSTRACT

We study a discrete model based on the observed behavior of excitable media. This model has the basic properties of an excitable medium, that is, a threshold phenomenon, a refractory period, and a globally stable rest point. We are mainly interested in two dimensional periodic patterns. We characterize the initial conditions which lead to such patterns, by introducing a basic invariant, the "winding number of a continuous cycle".

SIGNIFICANCE AND EXPLANATION

Pattern formation in living organisms is a basic problem in biology. Recently chemists have been studying certain (inorganic) chemical reactions which lead to interesting temporal and spatial patterns, in an effort to understand how such patterns arise. The interaction of diffusion and chemical reaction effects seems important. In this paper a discrete mathematical model is analyzed to see how these effects can lead to the sorts of behavior which have been seen experimentally.

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A GENERALIZATION OF ULTRASPHERICAL POLYNOMIALS

Richard Askey and Mourad E.-H. Ismail

Technical Summary Report #1851
May 1978

ABSTRACT

Some old polynomials of L. J. Rogers are orthogonal. Their weight function is given. The connection coefficient problem, which Rogers solved by guessing the formula and proving it by induction, is derived in a natural way and some other formulas are obtained. These polynomials generalize zonal spherical harmonics on spheres and include as special cases polynomials that are spherical functions on rank one spaces over reductive p-adic groups. A limiting case contains some Jacobi polynomials studied by Hylleraas that arose in work on the Yukawa potential.

SIGNIFICANCE AND EXPLANATION

Spherical harmonics are used to solve many physical problems, especially in potential theory. A generalization of zonal spherical harmonics was introduced by L. J. Rogers in 1895. He obtained many properties of these polynomials, including some that would not be found for the classical spherical harmonics for another twenty-five years. However he was unaware that his polynomials were orthogonal. The orthogonality relation is proved and used to obtain further results for these polynomials. Another limiting case gives a relatively recent result of Hylleraas that arose in his study of the Yukawa potential.

ABSTRACT

Interpolating elastica are the extremals for the functional $\int_0^{\bar{s}} \kappa^2(s)ds$, which is the integral of the square of the curvature with respect to arc length, in the family of plane curves that interpolate at (not prescribed) arc lengths $s_0 < s_1 < \ldots < s_n$ a prescribed configuration of points $P_0, P_1, \ldots, P_n$. If at one or both terminals the slope is prescribed, the extremal is said to be angle-constrained, otherwise free. The curvature functional represents the elastic strain energy of a thin elastic beam of indefinite length with sleeve supports anchored at $P_0, P_1, \ldots, P_n$, which allow the beam to slide through without friction and to rotate freely (except at the end supports if angle-constrained). The interpolating elastica are also known as nonlinear spline curves. It is known that the infimum of the strain energy is 0 in all cases, hence cannot be attained if the points $P_0, P_1, \ldots, P_n$ do not lie on a ray. On the other hand, interpolating elastica are known to exist for a variety of configurations, and this report investigates whether these extremals make the strain energy a local minimum or not (i.e. whether they are "stable" or "unstable"). Several general stability criteria are established and they are used to decide the stability of some specific elastica.

SIGNIFICANCE AND EXPLANATION

It is an old technique of draftsmen to use a mechanical spline to pass a smooth curve through a prescribed set of points in a plane. Curves which are obtained in this way (interpolating elastica, also called nonlinear spline curves) may be considered as the equilibrium positions of thin elastic beams which are constrained to pass through short, frictionless, freely rotating sleeve supports, anchored at the interpolation points. The strain energy of such a beam is given by the integral of the square of the curvature with respect to arc length, and equilibrium requires that the position be such that the energy be minimal for the given interpolation conditions. However, a global minimum cannot be attained (except in the trivial case of the unbent beam) since the energy can be made arbitrarily small by using sufficiently large loops between the supports. Instead one looks for local minima which guarantee stability against small perturbations. In this report some general stability criteria are established and some specific interpolating elastica are investigated for stability. Except for a few previous isolated observations these seem to be the first proven results on the stability of interpolating elastica.

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A RECURSIVE APPROACH TO PARAMETER ESTIMATION

IN REGRESSION AND TIME SERIES MODELS[†]

Johannes Ledolter

ABSTRACT

This paper discusses the recursive (on line) estimation of parameters in regression and autoregressive integrated moving average (ARIMA) time series models. The approach which is adopted uses Kalman filtering techniques to calculate estimates recursively. This approach can be used for the case of constant as well as time varying parameters.

In the first section the linear regression model is considered and recursive estimates of the parameters, both for constant and time varying parameters, are discussed. Since the stochastic model for the parameters over time will be rarely known, simplifying assumptions have to be made. In particular a random walk as a model for time varying parameters is assumed and it is shown how one can determine whether the parameters are constant or changing over time.

In the second section the recursive estimation of parameters in ARIMA models is considered. If moving average terms are present, the model has to be linearized and the Extended Kalman Filter can be used to recursively update the parameter estimates. The first order moving average model is discussed in detail.

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SIGNIFICANCE AND EXPLANATION

The problem discussed in this paper is the following: Observations up to time n (of, for example, business data or missile positions) are available and one wants to estimate unknown parameters in regression or autoregressive integrated moving average models in order to predict future values.

An additional observation is recorded. The question becomes how to update the parameter estimates from the previous estimates and the most recent observation without storing the complete past history of the data. The answer to this question will depend on whether the parameters in these models are assumed constant or whether they themselves follow a given stochastic process.

This recursive estimation procedure (which is sometimes called on-line estimation or parameter tracking) is important if the observations become available sequentially in time. It has applications in economics and business, where economic indicators and sales data are updated every week, month or quarter; it can also be applied to the control of satellites or ballistic missiles where the position in space is recorded every few seconds.

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A VARIATIONAL METHOD FOR FINDING PERIODIC SOLUTIONS
OF DIFFERENTIAL EQUATIONS

Paul H. Rabinowitz

Technical Summary Report #1854

May 1978

ABSTRACT

This paper concerns the use of minimax and approximation techniques from

the calculus of variations to prove the existence of periodic solutions of

Hamiltonian systems of ordinary differential equations. Most of the results

are for equations where the period is prescribed and assumptions are made about

the growth of the Hamiltonian near infinity. However it is also shown how such

results can give information about solutions having prescribed energy.

SIGNIFICANCE AND EXPLANATION

Hamilton's Principle gives a classical variational characterization of

a solution of Hamilton's equations as a critical point of an appropriate

functional. We develop a method here which is spiritually related to this

principle and which can be used to prove the existence of periodic solutions

to Hamilton's equations.

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A DRAZIN INVERSE FOR RECTANGULAR MATRICES

R. E. Cline† and T. N. E. Greville

Technical Summary Report #1855
June 1978

ABSTRACT

The definition of the Drazin inverse of a square matrix with complex elements is extended to rectangular matrices by showing that for any B and W, m by n and n by m, respectively, there exists a unique matrix, X, such that $(BW)^k = (BW)^{k+1}XW$, for some positive integer k, $XWBWX=X$ and $BWX = XWB$. Various expressions satisfied by B, W, X and related matrices are developed.

AMS(MOS) Subject Classification: 15A09

Key Words: Drazin inverse, rectangular matrix, weighted inverse

Work Unit No. 2 - Other Mathematical Methods

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SIGNIFICANCE AND EXPLANATION

Efficient methods for handling systems of linear simultaneous algebraic equations provide a fundamental tool in solving problems in almost every area of computing and applied mathematics. In matrix notation, the solution of $Ax = b$ is given by $x = A^{-1}b$, where A^{-1} denotes the inverse of A.

In classical matrix algebra, the inverse of A exists only if A is square and "nonsingular." The unique inverse then satisfies $AA^{-1} = A^{-1}A = I$. A singular or rectangular matrix has no inverse in this sense. However there may be associated with it a variety of "generalized inverses", each having some of the properties of the usual inverse. For example suppose that we have m equations in n unknowns, $Ax = b$, where A is $m \times n$, $m > n$, rank n. The solution in a least squares sense is

$$x = (A^T A)^{-1} A^T b$$

and the matrix multiplying b is a generalized inverse.

A certain type of generalized inverse, the Drazin inverse, has heretofore been defined only for square (usually singular) matrices and has found application to Markov processes and to the solution of systems of ordinary differential equations. In this paper the definition of the Drazin inverse is extended to rectangular matrices and its properties studied. (This extended Drazin inverse is defined in the Abstract.)

STRONG CONVERGENCE OF CONTRACTION SEMIGROUPS
AND OF ITERATIVE METHODS FOR ACCRETIVE OPERATORS
IN BANACH SPACES

Olavi Nevanlinna* and Simeon Reich**

ABSTRACT

Let A be an m-accretive operator in a Banach space E. Suppose that $A^{-1}0$ is not empty and that both E and E* are uniformly convex. We study a general condition on A that guarantees the strong convergence of the semigroup generated by -A and of related implicit and explicit iterative schemes to a zero of A. Rates of convergence are also obtained. In Hilbert space this condition has been recently introduced by A. Pazy. We also establish strong convergence under the assumption that the interior of $A^{-1}0$ is not empty. In Hilbert space this result is due to H. Brezis.

AMS(MOS) Subject Classifications: 47H05, 47H15, 65J05, 35B40.

Key Words: Semigroups of contractions, Iterative schemes, Uniformly convex
Banach spaces, Convergence rates.

Work Unit Number 1 - Applied Analysis

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SIGNIFICANCE AND EXPLANATION

This paper deals with two different but related topics: the behavior of evolution systems for large time, and finding zeros for certain operators. In [14] Pazy developed tools to analyze the behavior of some evolution systems. Here we show that these tools can be used in a more general setting and therefore the results can be applied to a larger set of problems. We then apply the same tools to problems where time has been discretized. This gives us iterative schemes for finding zeros for a large class of operators appearing both in physics and in convex programming. In particular we obtain detailed information on the rates of these iteration schemes.

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LANGUAGE REQUIREMENTS AND DESIGNS TO AID
DATA ANALYSIS AND STATISTICAL COMPUTING

Graham N. Wilkinson

Technical Summary Report #1857
June 1978

ABSTRACT

An outline is given of design requirements for high-level statistical computing languages, with special emphasis on nameable data-structures, general operations including matrix and table calculations, looping, branching and the use of macros, and on user-extendability. Implementation and evaluation are discussed briefly.

SIGNIFICANCE AND EXPLANATION

This report comprises an invited address to the International Statistical Institute at the 41st Session in West Delhi, India, December 1977, on the occasion of the inauguration of the new International Association for Statistical Computing.

In statistical data processing centers such as statistical departments of research institutes or government statistical offices, the major processing cost is in the preparation of computing tasks for the computer, particularly, when low-level languages like Fortran are used. Typically the preparation and programming costs exceeds the actual computing charges by a factor of something like ten or more, and these costs can be dramatically reduced by as much as 90% if sufficiently powerful high-level problem-oriented programming languages are available, for example the Genstat system in England and Australia, which accounts for a substantial fraction of all statistical computing in those countries. The paper addresses itself to the general design requirements for such high-level languages and their implementation.

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COMPUTABLE ERROR BOUNDS FOR THE NYSTRÖM METHOD

J. W. Hilgers[*] and L. B. Rall

Technical Summary Report #1858
June 1978

ABSTRACT

The classical Nyström method for the numerical solution of Fredholm
integral equations of second kind consists of numerical integration, colloca-
tion, and interpolation. The approximate solution obtained by this procedure
is shown to be identical to the solution of certain finite-rank integral
equations with kernels belonging to a specified class (K_n), and thus has
minimal error with respect to approximation of the original equation over
this class. A computable (but in general nonoptimal) error bound for the
Nyström approximate solution can be obtained on the basis of how well a
specific finite-rank integral operator with kernel in (K_n) approximates the
integral operator in the Fredholm equation being solved numerically.

AMS (MOS) Subject Classification: 65R05

Key Words: Nyström method, Fredholm integral equations, error estimation

Work Unit Numbers: 7 (Numerical Analysis) and 1 (Applied Analysis)

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SIGNIFICANCE AND EXPLANATION

Many problems in applied mathematics (such as boundary-value problems for
ordinary and partial differential equations) can be solved if a function $x(s)$
satisfying a Fredholm integral equation of second kind.

$$(1) \qquad x(s) - \lambda \int_0^1 K(s,t)x(t)dt = y(s), \qquad 0 \le s \le 1,$$

can be found, where $y(s)$ and $K(s,t)$ are known. In most cases, $x(s)$ can-
not be found explicitly, so numerical methods must be used. E. J. Nyström
developed a simple method of this type, using numerical integration to replace
the integral in (1) by the finite sum

$$\sum_{j=1}^n K(s,t_j)w_j z_j ,$$

where z_j are approximations to the values $x(t_j)$, the points $t_1, t_2, \ldots, t_n$
are the nodes and $w_1, w_2, \ldots, w_n$ the weights of the rule of numerical integra-
tion (Simpson, Gauss, etc.) being used. In order to determine the approximate
values $z_1, z_2, \ldots, z_n$, collocation at the points $t_1, t_2, \ldots, t_n$ is used to
obtain the system of equations

$$(2) \qquad z_i - \lambda \sum_{j=1}^n K(t_i,t_j)w_j z_j = y(t_i), \qquad i = 1,2,\ldots,n ,$$

to be solved for these values. Finally, interpolation by the formula

$$(3) \qquad z(s) = y(s) + \lambda \sum_{j=1}^n K(s,t_j)w_j z_j$$

gives an approximate solution of equation (1) on the entire interval $0 \le s \le 1$.
This method is simple in concept and easy to implement on electronic computers.
The question remains, how accurate are the results? In fact, the Nyström method
is known to produce good approximate solutions in many applications, but why is
this so? In this report, a number of ways of analyzing the accuracy of the
Nyström method are compared, and it is shown that error can be estimated by a
simple computational procedure based on approximation of $K(s,t)$ by kernels
of the form

$$(4) \qquad K_n(s,t) = \sum_{j=1}^n K(s,t_j)w_j v_j(t) .$$

It is also shown that the error of the Nyström method depends on the best possible
approximation of $K(s,t)$ by kernels $K_n(s,t)$ from a given class, and thus the
observed accuracy of this method has a theoretical explanation.

The responsibility for the wording and views expressed in this descriptive
summary lies with MRC, and not with the authors of this report.